

Diffusivity and Weak clustering in a Quasi 2D Granular Gas

J. A. Perera-Burgos^{1,2,*}, G. Pérez-Ángel^{1,2}, and Y. Nahmad-Molinari²

¹*Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados del IPN, Unidad Mérida, AP 73 “Cordemex”, 97310 Mérida, Yuc. México; and*

²*Instituto de Física “Manuel Sandoval Vallarta”,
Universidad Autónoma de San Luis Potosí,
Álvaro Obregón 64, San Luis Potosí, SLP, México*

(Dated: June 2, 2010)

Abstract

We present results from a detailed simulation of a quasi-2D dissipative granular gas, kept in a non-condensed steady state via vertical shaking over a rough substrate. This gas shows a weak power-law decay in the tails of its Pair Distribution Functions (PDF's), indicating fractality and therefore a tendency to form clusters over several size scales. This clustering depends monotonically on the dissipation coefficient, and disappears when the sphere-sphere collisions are conservative. Clustering is also sensitive to the packing fraction. This gas also displays the standard non-equilibrium characteristics of similar systems, including non-Maxwellian velocity distributions. The diffusion coefficients are calculated over all the conditions of the simulations, and it is found that diluted gases are more diffusive for smaller restitution coefficients.

PACS numbers: 47.70.Nd, 83.10.Rs

*Electronic address: jperera@mda.cinvestav.mx

I. INTRODUCTION

Two-dimensional (2D) granular gases have been widely studied as examples of out-of-equilibrium systems that are both simple enough to analyze and easy to construct experimentally. In the pioneering work of Olafsen and Urbach [1, 2] it was found that these gases, kept in a steady state via vertical shaking, could condensate into an hexagonal solid phase (for monodisperse sample) as the amplitude or frequency of shaking is reduced. This gives a fascinating example of fluid-solid transition not driven by molecular attraction or entropy maximization. In the gaseous phase, and confining the vertical expansion of the granular layer, the 2D Velocity Distribution Functions (VDFs) displayed by this system are non-Maxwellian, and tend to fall instead into an stretched exponential form. The deviation from Maxwellian behavior of the VDFs in granular gases has been studied theoretically [3–5], in simulations [6–12], and in experiments [2, 13–17], and have been characterized using Sonine polynomials [5, 17].

In its simpler form, experiments in granular gases are carried on using a horizontal cell with a perfectly flat bottom; due to dissipation, however, horizontal components of momentum tend to decrease and thus the gas finally undergoes an inelastic collapse into a static (with respect to the plane) condensed phase. In shaken experiments, for large vertical acceleration, and in the absence of vertical confinement, there is some dispersion in the instantaneous vertical position of the spheres, and the resulting off-plane collisions serve as a way of converting vertical momentum into horizontal momentum, keeping in this way the gas from condensing. This effect is large enough that it allows for the gas to keep some horizontal motion even in cases where a fraction of the beads never loose touch with the bottom [1]. In recent years some attempts have been made to provide mechanisms by which this transfer from vertical to horizontal momentum can be effected without depending on the fluctuations in height of the beads. For instance many theoretical and numerical models have been proposed based on an homogeneous granular gas randomly driven by a white noise [5, 18]. Experimentally, a complete layer of spheres glued to the bottom plate (the “floor”), or a first layer of heavy spheres on which a layer of light spheres is placed, have been used [15, 19], and in other cases an artificially roughened bottom plate was employed [17, 20]. It was found in these experiments that the behavior of the gas was somewhat closer to that of an ideal hard disk gas, including velocity distributions closer to the Maxwellian. The use of

a roughened substrate makes the movement of the particles to resemble Brownian motion, because of the frequent scatterings with the uneven floor.

Motivated by the experimental results reported in [20], in this paper we are describing a fully three-dimensional simulation of a confined vertically-shaken granular gas, where structure has been imposed in the bottom plate using fixed and non-overlapping small hemispheres. We find that this mechanism is quite efficient in avoiding the collapse of the gas into the quiescent state (that is, a state with no horizontal motion). We record the Mean Square Displacement (MSD) of the spheres in the gas, and study the dependence of the diffusion coefficient on packing fraction, adimensional acceleration and on restitution coefficient. We also report the obtained horizontal velocity distributions, and show the strong effects that friction with the upper confining plate (the “ceiling”) have in these functions. Finally we characterize the instantaneous state of the gas using its Pair Distribution Functions (PDF’s) [1, 2, 21–23], which give us information about the underlying effective interparticle interactions. We observe evidence of weak clustering in these PDFs, and relate them to the changes in diffusion in the system.

II. SIMULATION

We perform numerical simulations of a monodisperse granular gas of spheres in a quasi-bidimensional space, square with side L and with periodic boundary conditions in the horizontal. This gas is confined between two horizontal planes which oscillate in the vertical in a sinusoidal way $z = A \sin(\omega t)$, with amplitude A and frequency ω large enough so that the spheres will in general touch both confining plates in every oscillation of the system. In the bottom plate there are fixed and non-overlapping hemispheres whose diameter σ_{hs} is almost half of the diameter of the free spheres σ_s . These hemispheres move synchronously with the plane and are randomly distributed with a sufficiently high two-dimensional packing fraction ϕ_{hs} , so that no wide flat patches can be formed (see Fig. (1)). Here $\phi_{hs} = N_{hs}\pi\sigma_{hs}^2/(4L^2)$, where N_{hs} is the number of hemispheres in the plate of side L . The separation between planes is $h = 1.6\sigma_s + \sigma_{hs}/4 \approx 1.7\sigma_s$, and the minimum distance between the centers of two hemispheres is d_m .

In order to solve the Newton’s equations of motion we use standard time-driven molecular dynamics, using a velocity-Verlet integration with a predictor step for velocities. This is nec-

essary in order to incorporate the dissipative part of the force, which is velocity-dependent. The force between particles in contact is described by

$$\mathbf{F}_{ij} = \begin{cases} \mathbf{F}_{ij}^n + \mathbf{F}_{ij}^t & \text{when } \xi_{ij} > 0, \\ 0 & \text{otherwise,} \end{cases} \quad (1)$$

where \mathbf{F}_{ij}^n is a normal force which causes changes of the translational motion of the particles and \mathbf{F}_{ij}^t is a tangential force, originating in friction, which causes changes in both the translational and the rotational motion. The quantity ξ_{ij} is the mutual overlap (compression) of particles i and j and is defined by

$$\xi_{ij} = \max(0, \sigma_s - |\mathbf{r}_i - \mathbf{r}_j|) \quad (2)$$

for interparticle collisions, by

$$\xi_{ij} = \max(0, (\sigma_s + \sigma_{hs})/2 - |\mathbf{r}_i - \mathbf{R}_j|) \quad (3)$$

for particle-scatterer collisions, and by

$$\xi_{ip} = \max(0, \sigma_s/2 - d_{ip}) \quad (4)$$

for sphere-plate collisions. Here \mathbf{r}_i denotes the center of the i -th grain, \mathbf{R}_i the center of the i -th scatterer, and d_{ip} is the normal distance from the center of the i -th grain to the surface of the plate p .

Modeling a force that leads to inelastic collisions requires at least two terms: repulsion and some type of dissipation. The existing models and their characteristics, as well as comparisons among them, can be found in [24–29]. Here we have used for the normal force the linear spring-dashpot model, in which the contact interaction is modeled by the damped harmonic oscillator force

$$F_n = \min \left\{ 0, -\kappa_n \xi - \gamma_n \dot{\xi} \right\}, \quad (5)$$

where γ_n is a damping constant and κ_n is related to the stiffness of a spring whose elongations is ξ , the overlap between two grains (or a grain and a boundary plate). The advantage of this model lays in its analytic solution, where the collision time is given by

$$t_n = \pi \left(\frac{\kappa_n}{m_{\text{eff}}} - \left(\frac{\gamma_n}{2m_{\text{eff}}} \right)^2 \right)^{-1/2}, \quad (6)$$

and the restitution coefficient is

$$e_n = \exp \left(-\frac{\gamma_n}{2 m_{\text{eff}}} t_n \right). \quad (7)$$

Here m_{eff} is the effective mass for the colliding pair. For the tangential force we consider the Coulomb dynamical friction law $\mathbf{F}_{ij}^t = -\mu F_{ij}^n \hat{\mathbf{v}}_{i,j}^t$, where $\mathbf{v}_{i,j}^t$ is the unitary vector in the direction of the relative tangential velocity between spheres i and j (or, by extension, between a sphere and a scatterer or a sphere and a plate). The effect of gravity is incorporated into the vertical acceleration.

For the actual simulations we have taken most parameters similar to those of the previously mentioned experiments [20], as performed with steel spheres. Therefore, we have fixed the frequency of oscillation of the cell to $f = 60$ Hz, and have considered two amplitudes of oscillation: $A_1 = 0.024$ cm and $A_2 = 0.05$ cm, for every packing fraction ϕ of free spheres, getting in this way for the adimensional acceleration $\Gamma \equiv (2\pi f)^2 A/g$ the values $\Gamma_1 = 3.5$ and $\Gamma_2 = 7.2$. Here ϕ is defined as before by $\phi = N\sigma_s^2\pi/(4L^2)$. As parameters for the normal force, Eq. (5), we use those extracted from Eqs. (6,7), and fix the collision time to $t_n = 7.1 \times 10^{-5}$ s, and use three values of the restitution coefficients $e_n = 0.36, 0.66$ and 1 for the sphere-sphere and sphere-hemisphere interactions (at each value of Γ and for every packing fraction ϕ considered). The coefficient of restitution for sphere-substrate interaction was fixed at 0.878, corresponding to an experimentally measured steel-acrylic restitution coefficient [20], and the considered coefficient of dynamical friction μ was 0.25. The time-step of the integration is always fixed to $t_n/100$, and the simulation time is 40 s, after a transient of 10 s. The diameter of the free spheres σ_s and of the hemispheres σ_{hs} have been fixed to 0.44 cm and 0.2 cm, respectively, in all simulations. The minimal distance between hemispheres is $d_m = 0.2$ cm. Finally, the boundary plates have side $L = 16$ cm, and the packing fractions used have been $\phi = 0.15, 0.20, 0.25, 0.30$ and 0.35 for both Γ values used. The resulting numbers of grains are $N_s = 252, 336, 420, 504$ and 588 respectively, and the number of scatterers is $N_{hs} = 4100$. All the quantities reported here are the average over 10 simulations, each with a different configuration of hemispheres and different initial conditions.

III. NUMERICAL RESULT: DIFFUSION

We will start by presenting results for the diffusion in the quasi-2D granular gas. As mentioned before, the interaction with the hemispheres provides horizontal momentum to the particles, but also scatters their motion, making them to move on a pseudorandom way, resembling in certain form a Brownian motion. It is clear that the interparticle collisions also contribute to the scattering. In Fig. (2) we can see two trajectories for a single particle on a complete simulation of 40 s, one for the case with $e_n = 1$ and another for $e_n = 0.36$. This was done with a packing fraction $\phi = 0.15$, and the trajectory includes the interactions with the other particles and with the substrate. One must remember here that the restitution coefficient for particle-plate collisions is always fixed, while that for particle-hemisphere collisions is the same as the one for particle-particle collisions, and can be varied.

The MSDs measured fit very well the Einstein form

$$\langle (\mathbf{r}(t + t_0) - \mathbf{r}(t_0))^2 \rangle = 4 D t; \quad (8)$$

this is not as trivially expected as it may seem, since some recent results point to a breakdown of Einstein's law for 2D granular gases [30]. This is related to a well-known anomaly for self-diffusion in 2D, where the presence of hydrodynamical backflows gives origin to long tails in the velocity autocorrelation function. These tails behave as t^{-1} , giving in this way a logarithmic divergence to the diffusion coefficient, accordingly to the Green-Kubo formula [31, 32]. In our simulations we have not seen any evidence of non-Einsteinian behavior; in particular we have performed sets of longer runs (80 s) for three different sets of parameters, and one set of runs for a bigger system ($L = 16\sqrt{2} = 22.63$ cm), and in all cases the same diffusive behavior was found, with the diffusion coefficient independent of the length of the run or the system size. Looking at the difference between these results and those of [30], it is clear that the presence of fixed (with respect to the plane) scatterers is the reason why regular diffusion is restored.

In Fig. (3) we show the diffusion coefficient D versus the packing fraction for both values of the adimensional acceleration. Here we can observe the following points: first, D increases for low values of ϕ , and decrease for high values of ϕ . These results are in agreement with those obtained by [33, 34], and are to be expected, since larger densities represent in general more obstacles to the motion. Second, for small values of ϕ the diffusion coefficient increases when we lower e_n , and this behavior is stronger for low Γ . As the concentration and Γ grow,

this behavior reverses, that is, for large ϕ there is a crossover where the diffusion grows with e_n . Theoretical evidence for an inverse relationship between diffusion and restitution coefficients has recently been found in [33], as shown in their Fig. (5). This is also noticeable in our Fig. (2), where one can observe how the particle excursions are larger for lower e_n .

The increase in diffusion for smaller e_n is related to the appearance of density fluctuations that become stronger as the dissipation increases. This weak clusterization becomes apparent as a fall of the tails of the PDFs for large distances, as we will see later. Clusterization ends up freeing some space in the system, allowing in this way faster diffusion. The same phenomenon is well known in colloid-polymer mixtures, where the depletion forces induced by the (small) polymers create strong density fluctuations in the colloidal phase, and increase its diffusion [35, 36].

IV. GRANULAR TEMPERATURE AND VELOCITY DISTRIBUTION FUNCTIONS

In this section we perform a detailed analysis of the granular temperature T_g and of the Velocity Distribution Functions (VDFs) $P(v)$ obtained in the simulations. In Fig. (4) we can observe the behavior of the in-plane T_g , defined as $T_g = T_x + T_y = \langle v_x^2 \rangle + \langle v_y^2 \rangle$, as a function of the packing fraction ϕ , for all values of Γ and e_n considered. The following points deserve to be mentioned: first, for any given values of ϕ and e_n , T_g increases together with Γ , as is intuitively expected, and experimentally observed [17]. Second, one can observe that for given values of ϕ and Γ , T_g decreases together with e_n , also as expected. Third, and more interesting, we find that for $e_n = 1$ the T_g grows slowly with ϕ , in agreement with the experimental results obtained in [17]. In that experiment T_g grows monotonously until reaching a maximum for some $\phi_{\max} \approx 0.5$, and then decays as ϕ keeps growing. We do not find this later decay of T_g , probably because we are using values of ϕ below ϕ_{\max} .

The coincidence found for this particular value of e_n deserves some discussion: although the authors of [17] do not report their working value of e_n , other references [1, 37] give $e_n \approx 0.9$ for the stainless steel spheres used there. As relates to the simulation, we remind the reader that even when $e_n = 1$ there is some dissipation in our system, since this value of the restitution coefficient is applied only for sphere-sphere and sphere-hemisphere collisions. Contacts with the upper plate (and, even if infrequent, with the lower plate), are still

inelastic, with $e_n = 0.878$. Besides, the existence of a nonzero value of μ gives us some energy losses via friction, for all collisions. One may therefore assume that there is, in our simulation, some effective e_n a bit smaller than 1, and that the slow growth of the T_g for diluted gases found in both experiment and simulation occurs for high values of e_n , not necessarily $e_n = 1$. This should be stressed since, for values of e_n well below 1, T_g actually decays very slowly as ϕ increases, at least for the range of ϕ considered here. We are not aware of any experimental study of T_g for highly dissipative materials, and so there is no verification of this curious behavior reversal for small restitution coefficients.

The VDFs for both components of the horizontal velocity have been obtained, for all values of Γ , ϕ and e_n considered. In Fig. (5) we show a few of those curves, normalized by their characteristic velocities $v_c = \sqrt{\langle v_i^2 \rangle} = \sqrt{T_i}$. In the same Figure we also show, as a reference, a unitary Gaussian. The first remarkable fact is that for all values of ϕ , when $e_n = 0.66$ and 1.0 , with $\Gamma = 3.5$, and also for all values of e_n and $\Gamma = 7.2$, the VDFs present a strong peak at the center of the distribution—that is, for low velocities—. (Only some examples are shown, to avoid crowding the Figure.) These peaks can be also found in Fig. (8) of [17], for small ϕ . In that reference, they are attributed to the fact that at these packing fractions the effect of interparticle collisions is minimal, and so the general distribution is dominated by the VDF corresponding to one isolated particle. The simulations show that the main reason for the appearance of this peak is the friction of the grains with the upper plate in the system. In particular, as can be easily visualized in a 1D system, rotational velocities acquired at the collisions with the floor act as a braking factor upon contact with the ceiling, increasing in this way the concentration of particles with low horizontal velocities. In Fig. (6) we show the normalized curves for the VDFs, for the case $\phi = 0.20$, $\Gamma = 3.5$, and $e_n = 0.66$ and 1.0 , but taking the grain-ceiling value of μ as 0.0 in one case and $\mu = 0.25$ in the other. It is quite apparent from this Figure how, when there is no friction with the ceiling, there are no low-velocity peaks. However, it can be seen from the same Figure that the braking effect of the ceiling is not the only factor involved in the non-Gaussian behavior of the VDFs; in particular, the line for $e_n = 0.66$ and $\mu_{\text{ceiling}} = 0$ shows very clear deviations from the Gaussian. Even stronger deviations are found for $e_n = 0.36$ and $\mu_{\text{ceiling}} = 0$ (not shown in the Figure.) We would also like to mention that these peaks diminish as the packing fraction of the systems grows, as observed in [17].

To finish this section, let us show some analysis of the tails of the VDFs. In Figs. (7) and (8) we plot $-\log(-\log(P(v/v_c)/P(0)))$ vs. $\log(v/v_c)$ for $\Gamma = 3.5$ and $e_n = 0.36$, and for $\Gamma = 7.2$ and $e_n = 1.0$, as a function of ϕ . For a perfect Gaussian centered at the origin, this plot should give a straight line with slope $m = -2$. It can be observed from both Figures how the behavior of the tails of the VDFs change slowly with ϕ , but quite strongly as e_n is varied. We include in these graphs linear fits for the intermediate and final parts of the distribution. Here it is important to notice that for $\Gamma = 3.5$ y $e_n = 0.36$, both the intermediate and final parts of the VDFs are close to a Gaussian, as can be seen also, for $\phi = 0.15$, in Fig. (5). However, when $e_n = 1.0$, we find the intermediate and final parts of the distribution to be clearly different. While the final part is reasonably close to a Gaussian ($m_t \approx 2$) the intermediate part has an exponent larger than -1 . This is due to the effect of the ceiling, since the deformation of the VDFs—that is, their deviation from a Gaussian—in this region is related to the increase in the number of slow particles, which is in turn due to the friction with the upper plate. This general behavior can be corroborated in Fig. (8) ($\Gamma = 7.2$, $e_n = 1.0$). Here we can see how the final part of the distribution remains close to Gaussian, while one gets an exponent $m_t \approx -0.5$, much larger than -2 , for the intermediate part of the distribution.

One then finds that the effect of the rough substrate is to return the form of the VDFs to the Gaussian form, since the presence of the scatterers breaks translational symmetry and also forces a better horizontal energy interchange between the particles. On the contrary, the effect of the friction with the ceiling creates an increase in the distribution for slow particles, with a corresponding drop for the distribution at intermediate velocities.

V. PAIR DISTRIBUTION FUNCTIONS

The Pair Distribution Functions (PDFs) for a packing fraction $\phi = 0.35$ are shown in Fig. (9), for some combinations of Γ and e_n . It can be observed how when $e_n = 1$, the PDFs do not depend on Γ , and the structure observed is very similar to that of an equilibrium elastic hard sphere gas [2], indicating that the correlations that exist are mostly due to excluded volume effects. On the other hand, when the dissipation between particles increases, the correlations between particles begin to grow, an effect that is more notorious for low values of Γ .

The lines shown in the graph have two intriguing characteristics: first, we find a complete absence of any structure at $r/\sigma = \sqrt{3} = 1.73$, where a peak appears in the close-packed limit. Neither there is a peak around $r/\sigma = \sqrt{2} = 1.41$, which would signal some type of square clustering. It is therefore clear that the rough floor eliminates completely the possibility of formation of large crystalline clusters. Second, a very peculiar secondary peak develops, for small driving and high dissipation ($\Gamma = 3.5$ and $e_n = 0.36$), at $r/\sigma \approx 2$. The possible reason we have identified for the origin of this peak is the formation, at this low values of driving and restitution coefficient, of short-lived linear chains of grains (see Fig. (1) for an example). These linear chains may be induced by some residual order in the substrate, an order that in turn is due to the fact that it has to satisfy simultaneously a large density of scatterers and the no-overlap condition. It will be therefore interesting to see the evolution of $g(r)$ in those experiments where an ordered substrate has been used [15, 19]; although it is also clear from the graph that only for the smallest restitution coefficient used we get this peak.

For a more comprehensive view of the evolution of $g(r)$, in Fig. (10) we show the PDFs for $\Gamma = 3.5$, as a function of e_n and ϕ . The very strong effect that e_n has in these curves is the first thing to notice; for high dissipation the structure of the main peak in $g(r)$ is almost independent of ϕ , and little variation can be seen in the rest of the curve. The large value of $g(r)$ at the main peak signals a tendency to clustering. At the other extreme, the gas with $e_n = 1.0$ shows much more sensitivity to ϕ . An unusual behavior can be seen for $e_n = 1$ and small ϕ : the largest value of $g(r)$ no longer falls at contact, and instead, a soft “hill” develops around $r/\sigma \approx 1.2$ – 1.3 . This is again an effect of the scatterers, that at this high value of e_n intrude between the grains, and, for small packing factors, reduce the probability of contact. Again, there is no signal of any peak at $r/\sigma = \sqrt{3}$, but we find instead that for the most dissipative system, some peak at $r/\sigma = 2$ begins to form. Visual inspection of the dynamics in this parameter sector shows in effect the presence of short-lived linear chains. For $\Gamma = 7.2$ (not shown) the results found are analogous: there is an increase in the height of the main peak of $g(r)$ as e_n is lowered, although not as strong as for $\Gamma = 3.5$; and there is absolutely no peak at $r/\sigma = \sqrt{3}$. As for the behavior around $r/\sigma = 2$, now only some weak increase in $g(r)$ can be detected. A remarkable result is the fact that for all ϕ used the different $g(r)$ obtained for $e_n = 1$ agree completely for both values of Γ .

Finally, one of the most interesting points in the phenomenology of this granular gas is shown in Fig. (11), which displays a close up to the PDFs for $\Gamma = 3.5$. It can be observed

here that for each filling fraction considered, $g(r)$ has its long- r tail falling slightly below 1.0 when we lower the restitution coefficient, something that does not happen in the curves with $e_n = 1$. We would like to stress that the same normalization protocols were used for all lines. This behavior implies a weak fractal behavior related to the non-unitary restitution coefficients in the system. More in detail, one can observe that the tails in the PDFs show the largest drop below 1.0 for $\phi = 0.15$ and $e_n = 0.36$; in general, the PDFs approach 1.0 from below as ϕ increases or e_n increase. As an effect of the clusterization signaled by the falling of the PDFs below 1, there is an increase in the mean free path of those particles outside of the clusters—that is, in the more diluted part of the gas—. This gives rise to an increase of the average diffusion coefficient of the system, as was shown in Fig. (3). For $\Gamma = 7.2$ one gets some appreciable decay in the tails of $g(r)$ only for small ϕ and small e_n , and in general this effect is not so strong. This behavior again coincides with the increase in diffusion found for this value of Γ , as can be seen in Fig. (3).

It is important to notice that the decay observed in the tails of the PDFs is due only to interparticle collisions, and independent of friction, either with the floor or the ceiling. This can be observed in Fig. (11), where the fastest decay of the tails of the $g(r)$ appears for $\Gamma = 3.5$ y $e_n = 0.36$; for these values of the parameters the VDFs are practically Gaussian, as can be seen in Fig. (5), implying very little interaction with the ceiling.

So, it is clear, looking at the results for diffusion and for the PDFs, that clustering increases the average diffusion, even if these clusters are very unstable and their lifetimes are very short. The weakly fractal behavior of the gas disappears when we increase any of the three controlling parameters in the system: the packing fraction, the amplitude of vibration or the restitution coefficient.

VI. CONCLUSIONS AND FINAL COMMENTS

We have performed numerical simulations of a vibrating quasi 2D granular gas, using a fully 3D algorithm with Coulomb friction proportional to normal forces, for a horizontal granular gas confined by a rough floor and a flat ceiling. The system shows some of the characteristics already explored in experimental and other simulational work, as for instance the recovery of Gaussian VDFs at low Γ over a rough substrate. The principal result of the simulation is how, even with a floor full of scatterers, there is some level of clustering for

the low range of Γ , e_n and ϕ values. This clustering shows in the strong growth of the main peak of $g(r)$, in the increase in diffusivity as e_n is lowered, and very clearly in the drop of $g(r)$ below 1 for $r \gg \sigma$. All of the characteristics that indicate clustering coexist, however, with an almost complete recovery of Gaussian behavior in the VDFs for this part of the parameter space. For the other corner of this space—that is, high Γ and ϕ and $e_n = 1$ —all signals of clustering disappear, making it clear that the rough floor is only of minor importance with respect to this behavior.

There are also some very punctual phenomena associated to this simulation: first, it shows quite dramatically the distorting effect that the ceiling may have on the VDFs, by introducing a braking affect that results in a large increase in the central part of the distributions—the very low velocity regime—. Experimental results reported up to now show some hints of this problem, but there is not, to our knowledge, any systematic experimental exploration of this effect. Also, the presence of a peak in $g(r)$ around $r/\sigma = 2$ is pointing towards some complex effects of the substrate on the dynamics. Even if the configurations of scatterers used in the simulation have a random origin, the simultaneous demands large density and no overlap may have introduced some level of ordering, later reflected is a larger-than-expected population of linear and almost-linear chains in the granular gas. The appearance of undesired order in the substrate is not surprising, since it is actually quite difficult to pack monodisperse disks densely without generating a crystal.

Acknowledgments

This work was supported by CONACyT (Mexico) through Grant No. 82975. J. A. P.-B. receives support from a CONACyT Doctorate Fellowship.

-
- [1] J. S. Olafsen and J. S. Urbach, Phys. Rev. Lett. **81**, 4369 (1998).
 - [2] J. S. Olafsen and J. S. Urbach, Phys. Rev. E **60**, R2468 (1999).
 - [3] A. Puglisi, V. Loreto, U. Marini Bettolo Marconi and A. Vulpiani, Phys. Rev. E **50**, 5582 (1999).
 - [4] N. V. Brilliantov and T. Pöschel, Phys. Rev. E **61**, 5573 (2000).
 - [5] T. van Noije and M. Ernst, Granular Matter **1**, 57 (1998).

- [6] Y. H. Taguchi and H. Takayasu, Europhys. Lett. **30**, 499 (1995).
- [7] X. Nie, E. Ben-Naim and S. Y. Chen, Europhys. Lett. **51**, 679 (2000).
- [8] A. Barrat and E. Trizac, Phys. Rev. E **66**, 051303 (2002).
- [9] J. S. van Zon and F. C. MacKintosh, Phys. Rev. Lett. **93**, 038001 (2004).
- [10] J. S. van Zon and F. C. MacKintosh, Phys. Rev. E **72**, 051301 (2005).
- [11] D. J. Bray, M. R. Swift and P. J. King, Phys. Rev. E **75**, 062301 (2007).
- [12] A. Burdeau and P. Viot, Phys. Rev. E **79**, 061306 (2009).
- [13] W. Losert, D. G. W. Cooper, J. Delour, A. Kudrolli and J. P. Gollub, CHAOS **9**, 682 (1999).
- [14] A. Kudrolli and J. Henri, Phys. Rev. E **62**, 1489 (2000).
- [15] A. Prevost, D. A. Egolf and J. S. Urbach, Phys. Rev. Lett. **89**, 084301 (2002).
- [16] K. Kohlstedt, A. Snezhko, M. V. Sapozhnikov, I. S. Aranson, J. S. Olafsen and E. Ben-Naim, Phys. Rev. Lett. **95**, 068001 (2005).
- [17] P. M. Reis, R. A. Ingale and M. D. Shattuck, Phys. Rev. E **75**, 051311 (2007).
- [18] D. R. M. Williams and F. C. MacKintosh, Phys. Rev. E **54**, R9 (1996).
- [19] G. W. Baxter and J. S. Olafsen, Nature **425**, 680 (2003).
- [20] R. A. Bordallo-Favela, A. Ramírez-Saíto, C. A. Pacheco-Molina, J. A. Perera-Burgos, Y. Nahmad-Molinari and G. Pérez-Ángel, Eur. Phys. J. E **28**, 395 (2009).
- [21] B. V. R. Tata, P. V. Rajamani, J. Chakrabarti, A. Nikolov and D. T. Wasan, Phys. Rev. Lett. **84**, 3626 (2000).
- [22] P. Eshuis, K. van der Weele, D. van der Meer and D. Lohse, Phys. Rev. Lett. **95**, 258001 (2005).
- [23] F. Páchecho-Vázquez, G. A. Caballero-Robledo and J. C. Ruiz-Súarez, Phys. Rev. Lett. **102**, 170601 (2009).
- [24] J. Schäfer, S. Dippel and D. E. Wolf, J. Phys. I. France **6**, 5 (1996).
- [25] N. V. Brilliantov, F. Spahn, J.-M. Hertzsch and T. Pöschel, Phys. Rev. E **53**, 5382 (1996).
- [26] A. Di Renzo and F. P. Di Maio, Chemical Engineering Science **59**, 525 (2004).
- [27] A. B. Stevens and C. M. Hrenya, Powder Technology **154**, 99 (2005).
- [28] H. Kruggel-Emden, E. Simsek, S. Rickelt, S. Wirtz and V. Scherer, Powder Technology **171**, 157 (2007).
- [29] T. Pöschel and T. Schwager, *Computational Granular Dynamics: Models and Algorithms* (Springer, 2004).

- [30] C. Henrique, G. Batrouni and D. Bideau, in *Granular Gases*, edited by T. Pöschel and S. Luding, Lecture Notes in Physics vol. 564, p.140.
- [31] B. J. Alder and T. E. Wainwright, Phys. Rev. A **1** 18 (1970).
- [32] P. J. Camp, Phys. Rev. E **71** 031507 (2005).
- [33] W. T. Kranz, M. Sperl and A. Zippelius, arXiv:1002.2150v1.
- [34] A. R. Abate and D. J. Durian, Phys. Rev. E **74** 031308 (2006).
- [35] K. N. Pham *et al.*, Science **296** 104 (2002).
- [36] R. Juárez-Maldonado and M. Medina-Noyola, Phys. Rev. E **77** 051503 (2008).
- [37] A. Kudrolli, M. Wolpert and J. P. Gollub Phys. Rev. Lett. **78** 1383 (1997).

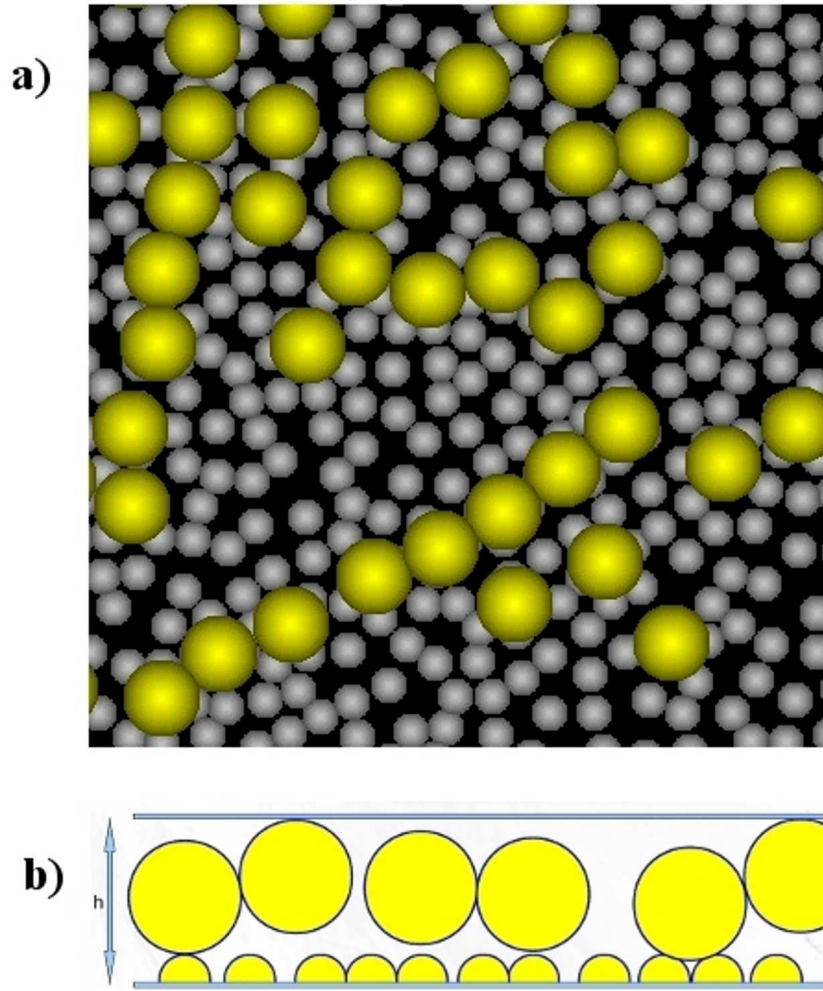


FIG. 1: (a) Fraction of a snapshot (taken from above) of the granular gas, covering around $1/13$ of the actually simulated area. The hemispheres (scatterers) are shown as white circles, the moving grains as yellow circles. Notice the presence of some short linear chains. (b) Schematic lateral view of the simulated system, to scale.

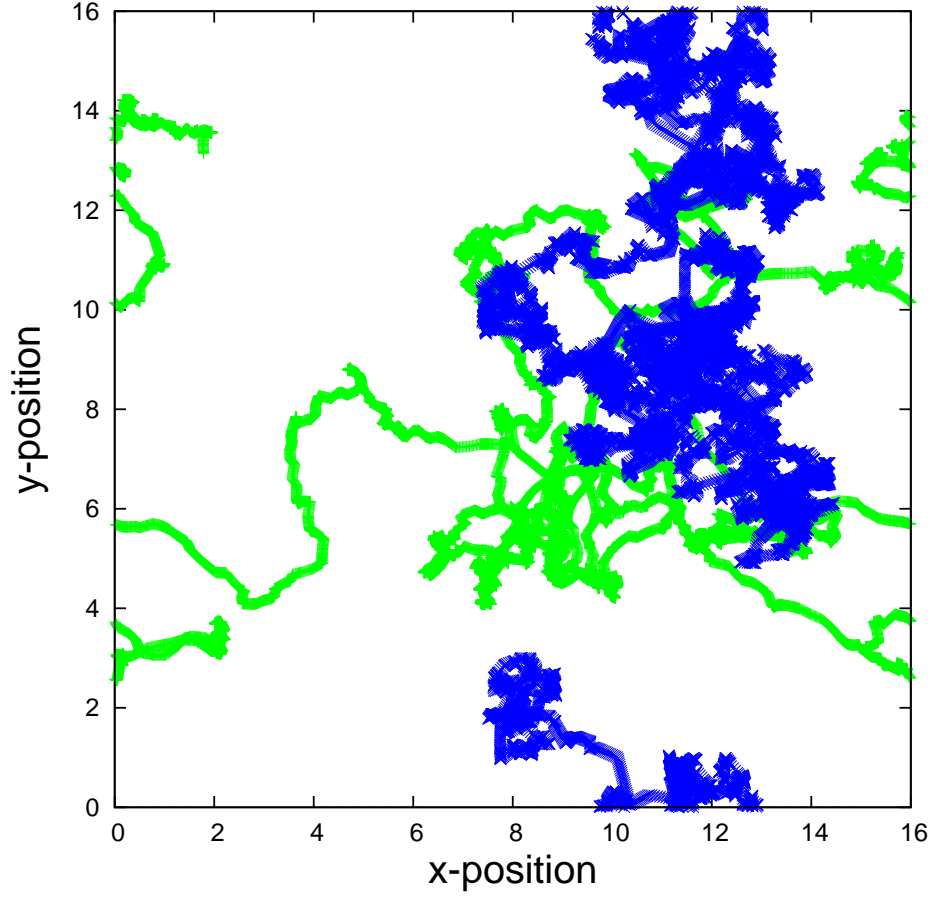


FIG. 2: Trajectory of a single particle for two different restitution coefficients. The more compact trace (blue) is for $e_n = 1.0$, the less compact one (green) is for $e_n = 0.36$. The packing fraction is 0.15 and we used $\Gamma = 3.5$. Notice how the tracer describes a much larger excursion for the smaller restitution coefficient.

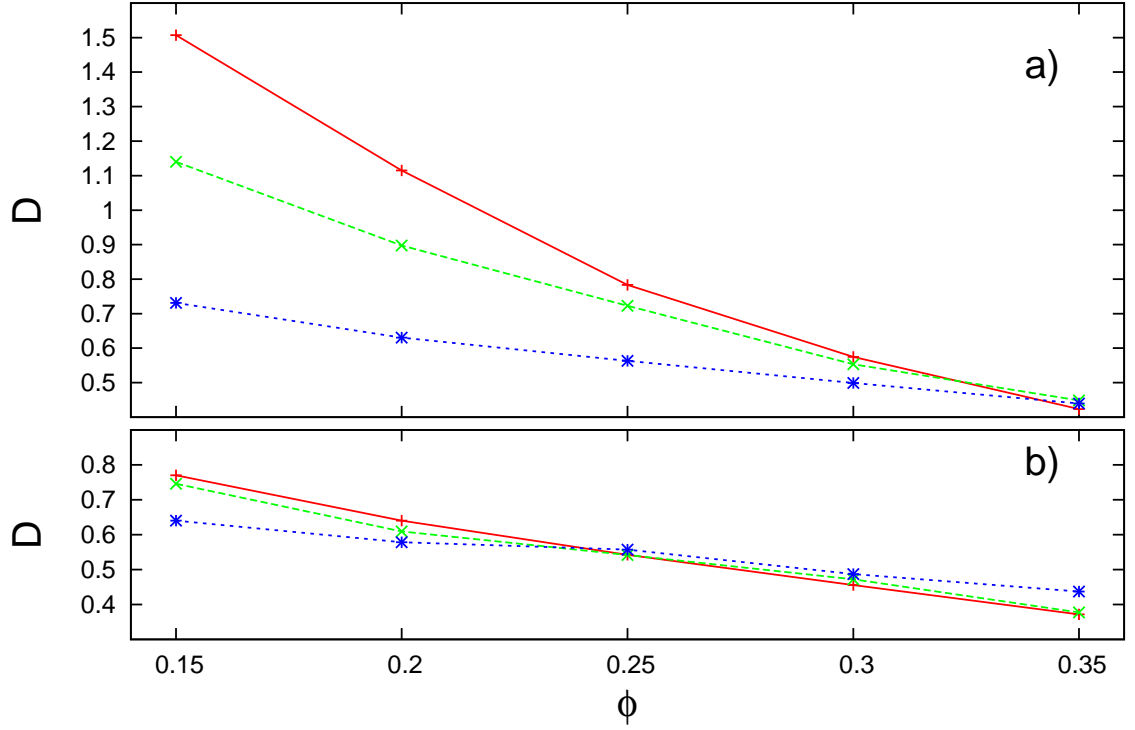


FIG. 3: Diffusion Coefficients vs Filling Fraction for: (a) $\Gamma = 3.5$, and (b) $\Gamma = 7.2$. The values of e_n are, at the left and starting from top: $e_n = 0.36$ (red), $e_n = 0.66$ (green) and $e_n = 1$ (blue). For the range of packing fractions covered, D always decreases with ϕ . The behavior with respect to e_n is more complex: for small ϕ , D decays as e_n grows. For large ϕ there seems to be a crossover where D starts growing with e_n .

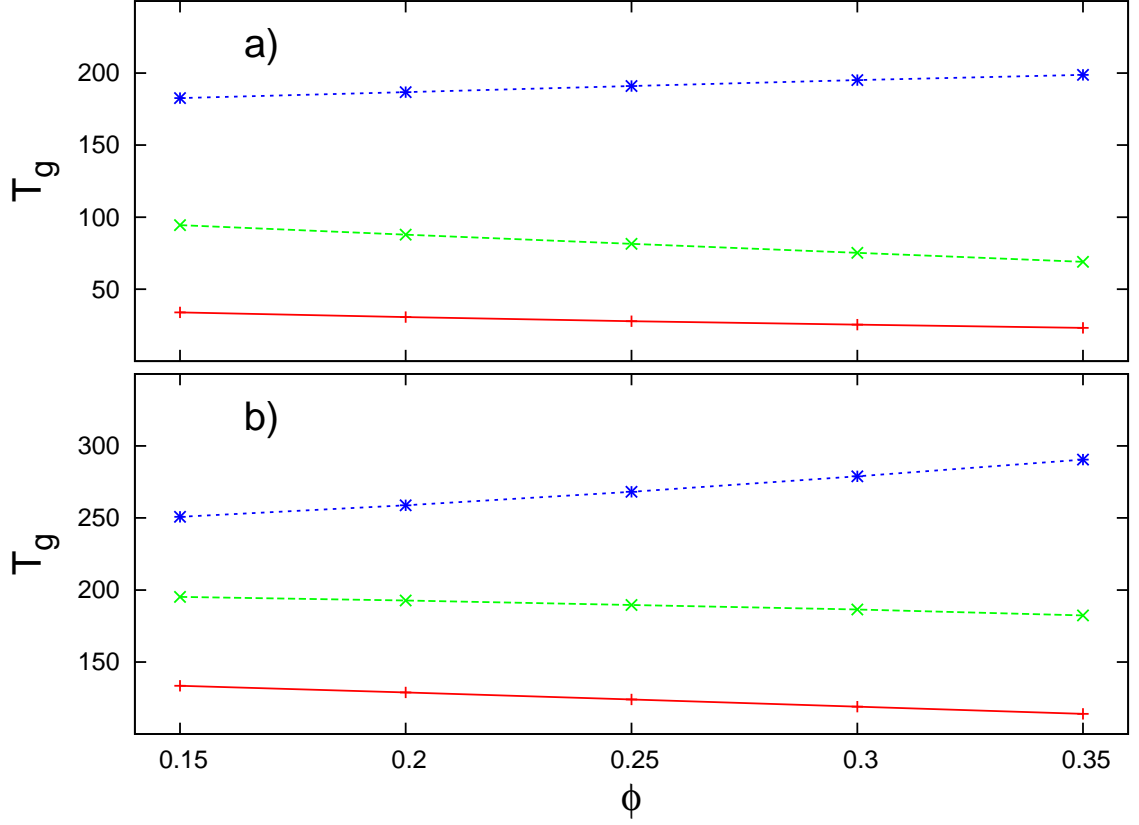


FIG. 4: T_g vs ϕ for both values of (a) $\Gamma = 3.5$ and (b) $\Gamma = 7.2$. The values of e_n are, for both graphs and starting from top: $e_n = 1$ (blue), $e_n = 0.66$ (green), $e_n = 0.33$ (red). The dependence of T_g on ϕ is much weaker than its dependence on e_n . For both values of Γ we find T_g decaying slowly with ϕ at low values of e_n , but increasing, again slowly, with ϕ for $e_n = 1$.

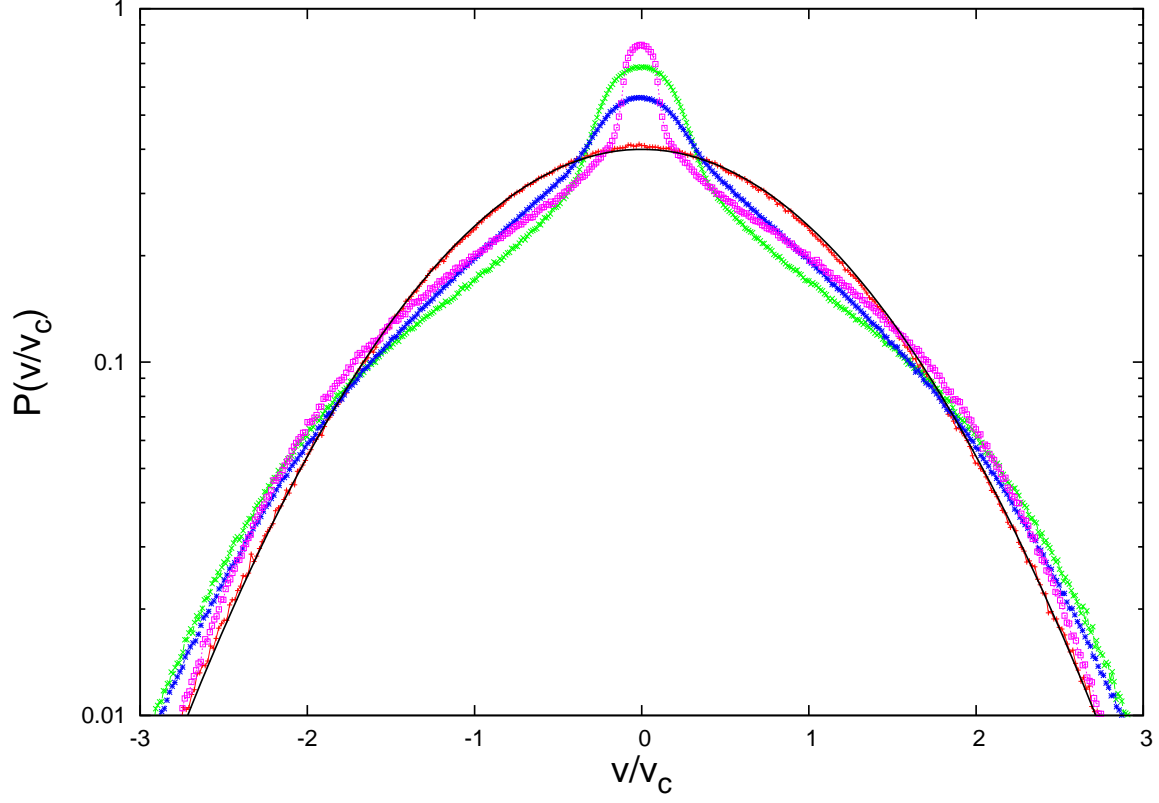


FIG. 5: Velocity Distribution Functions (VDFs) for some values of the parameters. Here the VDFs have been scaled by the RMS velocity. Looking at the center, and starting from the top, the four thick lines correspond to: $\Gamma = 7.2$, $\phi = 0.15$ and $e_n = 0.36$ (magenta); $\Gamma = 3.5$, $\phi = 0.15$ and $e_n = 1.0$ (green); $\Gamma = 3.5$, $\phi = 0.35$ and $e_n = 1.0$ (blue); and $\Gamma = 3.5$, $\phi = 0.15$ and $e_n = 0.36$ (red). The thin black line corresponds to a Gaussian distribution. For the last set of parameters the combination of high dissipation and small Γ results in trajectories where the grains almost never touch the ceiling, giving therefore a VDF very close to the Gaussian.

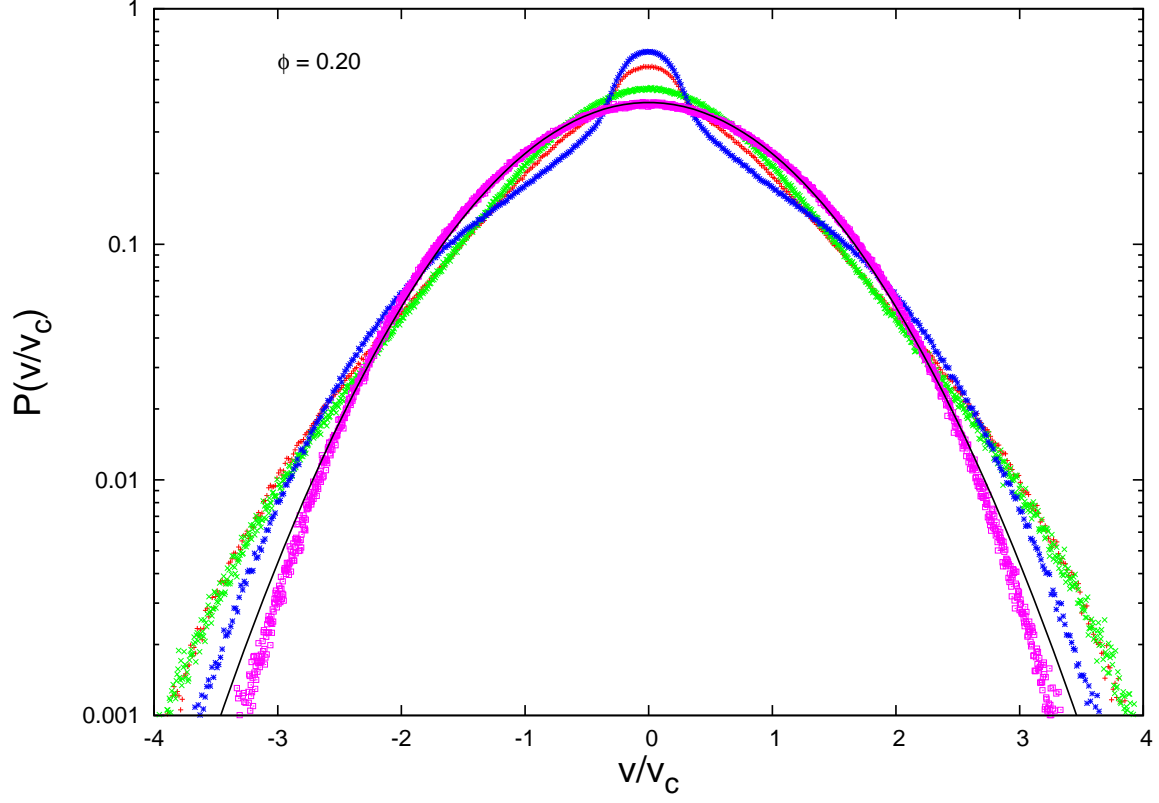


FIG. 6: Some VDFs with and without friction with the ceiling. For all lines we have used here $\Gamma = 3.5$ and $\phi = 0.2$. Looking at the center, and starting from the top, the four thick lines correspond to (a) $e_n = 1.0$ and $\mu = 0.25$; (a) $e_n = 0.66$ and $\mu = 0.25$; (a) $e_n = 0.66$ and $\mu = 0$; and (a) $e_n = 1.0$ and $\mu = 0$. The thin black line is again a Gaussian distribution.

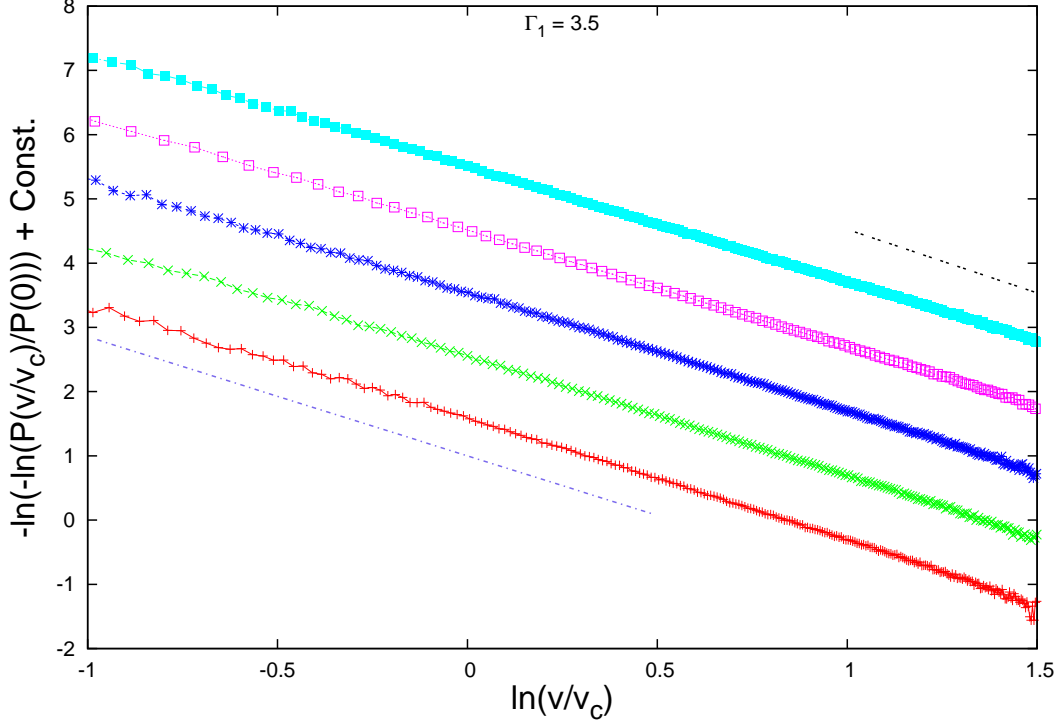


FIG. 7: Intermediate and outer parts of the VDFs for $\Gamma = 3.5$ and $e = 0.36$, for different values of ϕ . Starting from top, the values of ϕ are 0.15, 0.20, 0.25, 0.30, 0.35. For clarity, lines have been shifted apart from each other. Again, low Γ and e_n reduce contacts with the ceiling, therefore generating VDFs very close to Gaussians. The slope m in the intermediate region is $m = -1.85$ (thin blue segment), and for the outer region (the tails) we get $m = -1.97$ (thin black segment).

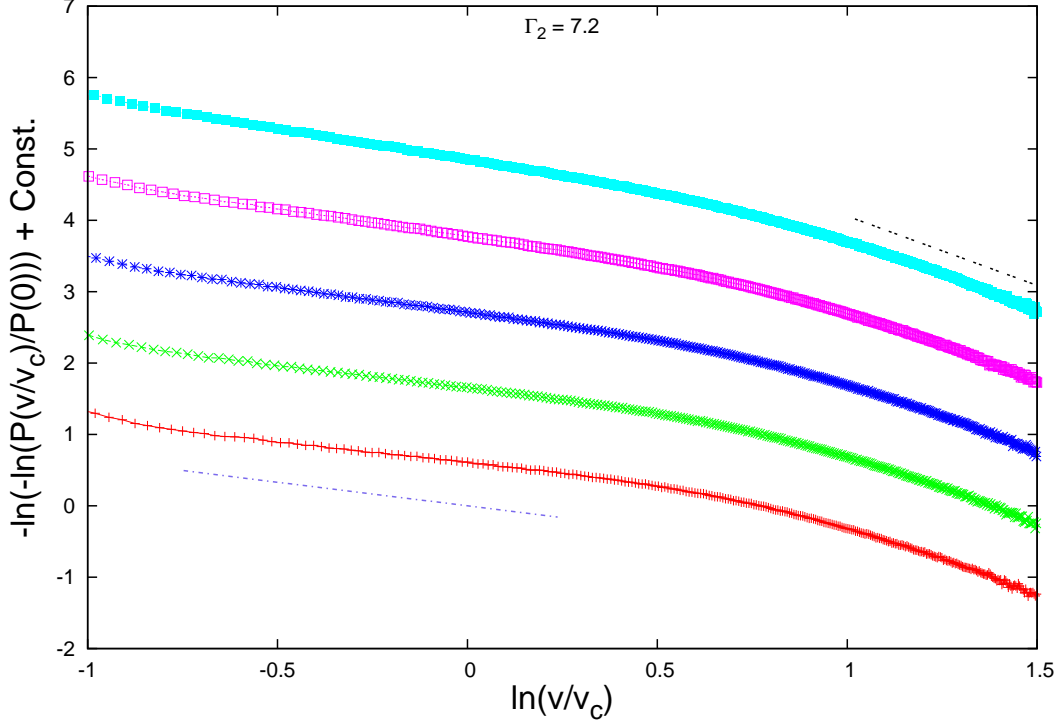


FIG. 8: Intermediate and outer parts of the VDFs for $\Gamma = 7.2$ and $e = 1.00$, for different values of ϕ . The values of ϕ are as in the previous Figure, and again the lines have been shifted apart from each other. Here the high Γ and e_n imply strong bounces in the ceiling, and therefore a very noticeable shift of the VDF towards low velocities. These VDFs are quite distorted, and the double-log vs log graph cannot be fitted well with straight lines. The best linear fits for the intermediate and outer regions give $m = -0.66$ (thin blue segment) and $m = -1.94$ (thin black segment), respectively.

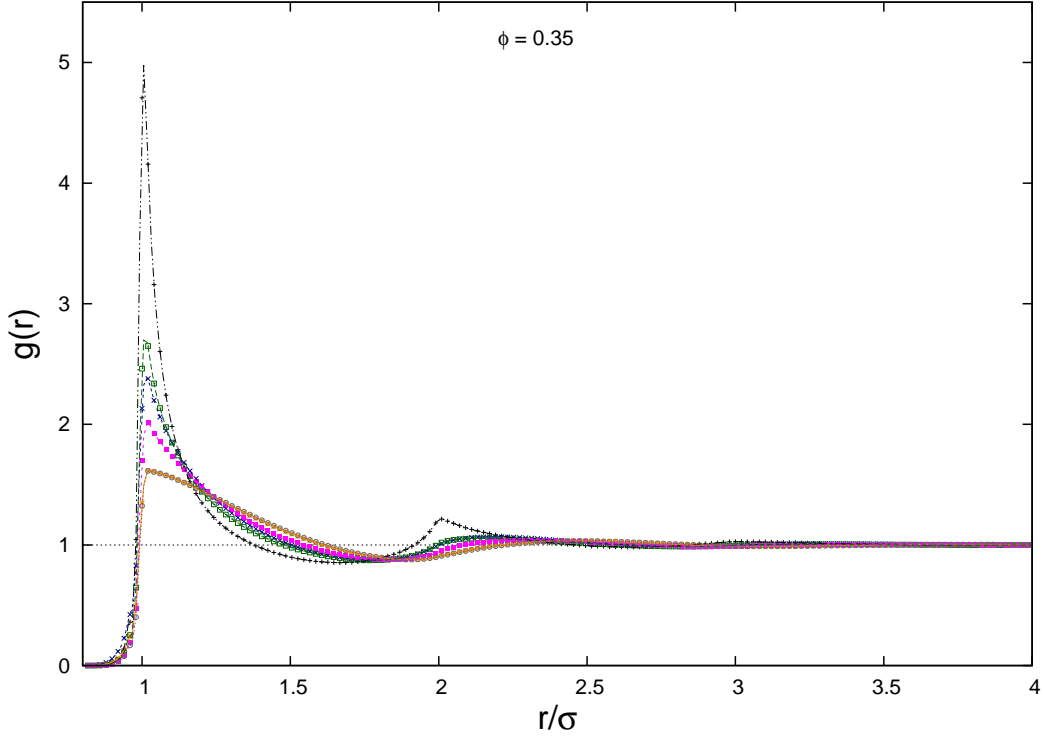


FIG. 9: Pair distribution functions for $\phi = 0.35$ for some values of Γ and e_n . At the main peak, and starting from top, the changing parameters are: (a) $\Gamma = 3.5$, $e_n = 0.36$; (b) $\Gamma = 7.2$, $e_n = 0.36$; (c) $\Gamma = 3.5$, $e_n = 0.66$; (d) $\Gamma = 7.2$, $e_n = 0.66$; (e) $\Gamma = 3.5$, $e_n = 1.0$ and (f) $\Gamma = 7.2$, $e_n = 1.0$. The last two lines fall on top of each other, showing how the PDFs for non-dissipative grains are independent of the acceleration. In general, smaller restitution coefficients give rise to larger values of $g(r)$ at contact.

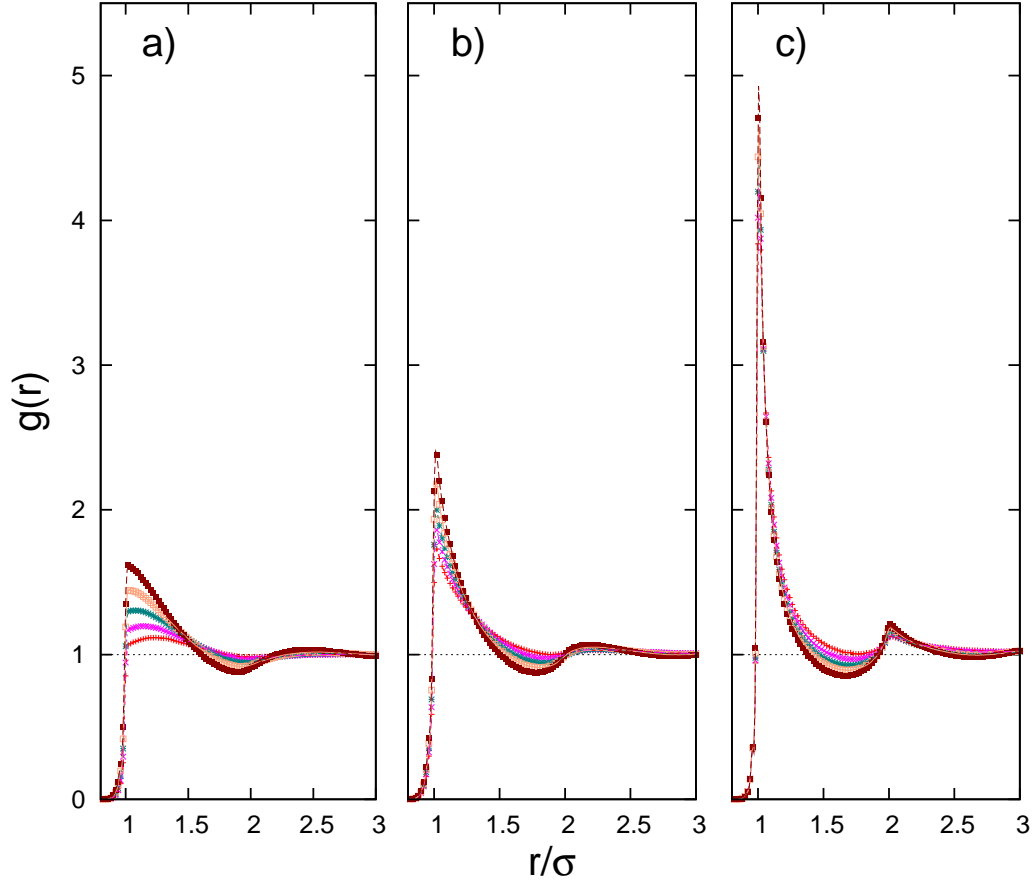


FIG. 10: Pair distribution functions for $\Gamma_1 = 3.5$, for: (a) $e_n = 1.0$, (b) $e_n = 0.66$, and (c) $e_n = 0.36$. In all cases, the $g(r)$ with the largest variation corresponds to $\phi = 0.35$, and $g(r)$ becomes progressively flatter as ϕ decreases. Notice that in (a), for $\phi < 0.30$, the largest peak is not located at contact, indicating that the fixed scatterers have a weak separating effect over the grains.

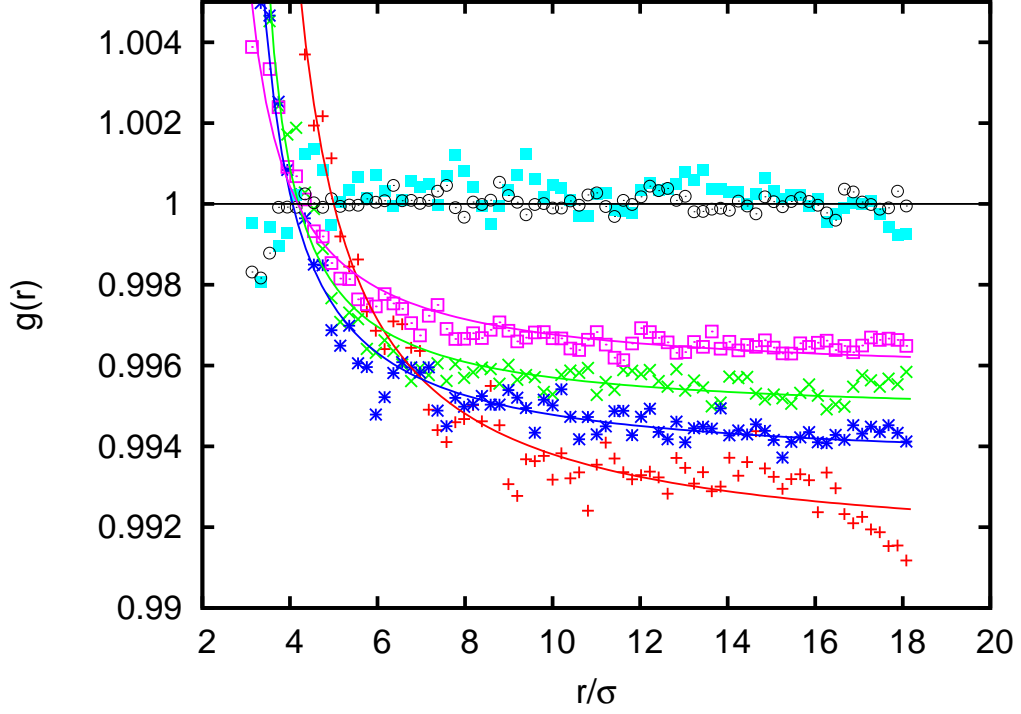


FIG. 11: Zoom of the $g(r)$ for $\Gamma_1 = 3.5$. The decreasing of the $g(r)$ tails can be observed for different filling fractions with respect to the curve with $e = 1$. The parameters are, starting from below: (a) $e_n = 0.36$, $\phi = 0.15$ (red), (b) $e_n = 0.66$, $\phi = 0.15$ (blue), (c) $e_n = 0.36$, $\phi = 0.25$ (green), and (d) $e_n = 0.66$, $\phi = 0.25$ (magenta). The two sets of points running at $g(r) = 1$ correspond to $e_n = 1$, for $\phi = 0.15$ and 0.25 . The lines are fits of the form $y(x) = A + B/(x - x_0)$, and are provided only as guides to the eye; at this reduced vertical scale, the large noise levels in the data make a detailed evaluation of the parameters of the fit too uncertain as to be useful.